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Evaluation of the Material Point Method within CTH to Model 2-Dimensional Plate Impact Problems

by Denzell Bolling

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14. ABSTRACT
The material point method (MPM) is a mixed Eulerian and Lagrangian computational method that allows for the discretization of solid bodies into material points carrying the full material state of the original body. This method is being evaluated as a new implementation within CTH, a code originally developed by Sandia National Laboratories, as a way of eventually dealing with fracture and other difficult solid mechanics scenarios. Applying CTH with MPM to a 2-dimensional plate impact problem yields multiple issues that must be examined. Issues with void compression upon initial impact, inhomogeneous particle states within a single cell, and inconsistencies within results obtained at different mesh resolutions are all discussed.

15. SUBJECT TERMS
impact, particles, CTH, markers, material point method, particle in cell

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Student Bio

I am currently attending Howard University in Washington, DC, as a second-year graduate student within mechanical engineering. I also attended Howard University for my undergraduate degree in mechanical engineering. My past research experience includes an internship at Sandia National Laboratories studying the expansion of oil reserve reservoirs. I also worked on 2 undergraduate research experiences at the Georgia Institute of Technology studying alternative energy. In the future, I plan on finishing my master’s degree and applying for PhD programs within mechanical engineering.

1. Introduction/Background

CTH is a continuum hydrocode originally developed by Sandia National Laboratories. The software system can model multidimensional, multimaterial, large deformation, and strong shock wave physics.[1] The existing code is used widely across the US Army Research Laboratory; increasing the code's capabilities would be a great benefit. For example, in cases that involve material fracture, continuum Eulerian codes such as CTH do not track fractures cleanly and can smear cracks and change their extent or growth characteristics. These adverse numerical artifacts can introduce error into computational results.[2]

The recent implementation of the material point method (MPM) into CTH may ameliorate some of these difficulties. This method involves the discretization of solid bodies into Lagrangian material points. These points (also called markers) carry the full state of the material, including mass, density, velocity, stress, and strain. Interactions among adjacent cells of the numerical background grid enforce compatibility and momentum balance, and the constitutive relations are evaluated on the markers. The markers receive their strain rate from the continuum grid during the Lagrangian part of the step, and the stress and material history are updated for the markers. The material points remain fixed to the material as the grid is returned to its original spatial location during a remap step. The remapped markers provide the stress to the grid for the momentum calculation to complete the cycle. The transient coupling between the particles and the grid enables large deformations of the Lagrangian particles without mesh tangling. Simply stated here, the inclusion of MPM has the potential to assist in accurately solving all kinds of large deformation mechanics problems where the internal state of material is history dependent.[3]

The incorporation of MPM within CTH creates a new capability to be evaluated within this report. One of the central differences between continuum CTH and CTH with MPM is the superposition of 2 separate pressure terms within the momentum equation (Eq. 1) used in the analysis.[4]

$$\Delta \boldsymbol{u} = \frac{\Delta t}{m_s}\int -\nabla\cdot(P\boldsymbol{I}+\boldsymbol{Q})dV + \frac{\Delta t}{m_s}\int \nabla\cdot(\boldsymbol{\sigma}_s + P\boldsymbol{I})dV + \frac{\Delta t}{m_s}\int \rho_s \boldsymbol{b}\, dV \ . \tag{1}$$

This equation can be broken down into 3 terms. The first term is the continuum term; it is the traditional way of computing accelerations induced by the pressure gradient on the background grid. The second term is the particle term; it holds the full stress tensor, $\boldsymbol{\sigma}_s$, at the particle level. The third term is a body force term, which does not play a role in the following computations. The additive contributions of the positive pressure at the particle level and the negative pressure at the continuum level play a significant role in how CTH with MPM computes acceleration of the grid. In a uniform field, the pressure contribution removed from the particle term is exactly replaced by the continuum pressure from the background grid. For inhomogeneous

deformation fields, the result is more complex, as will be suggested in this work. A thorough understanding of the CTH solution algorithm with markers will lead to greater confidence for using the markers in a wide range of Army problems.

2. Experiment/Calculations

The evaluation of CTH with MPM is conducted on 2 main levels. The first level is a direct response comparison of CTH with and without particles for a zero-obliquity impact problem between 2 similar materials. The second level of the evaluation investigates mesh sensitivity for the particle models using 2 different mesh resolutions, one fine and another coarse. A comparison between these 2 resolutions ensures that the code is converging to a physically reasonable solution based on different levels of mesh refinement. Comparisons between the different paired simulations briefly described here demonstrate how accurately the new capabilities of CTH operate. The input deck built for these tests is composed of multiple components, including the mesh, diatom, markers, tracers, and the equation of state needed to compute the stress state of the materials.

2.1 Mesh

The mesh is a user-supplied spatial discretization of the material geometries for the problem of interest. For a Lagrangian domain, the mesh moves with the material, and for a Eulerian domain, the material advects through a stationary mesh. Mesh creation for the current evaluation uses a Eulerian domain with a 2-dimensional (2-D) rectangular geometry. Its mesh extends from –0.01 to 0.01 m along the flyer plate propagation direction. There are 400 elements of 5×10^{-5} m dimension for the fine mesh and 100 elements of 2×10^{-4} m dimension for the coarse mesh. The mesh extends 0.002 m from the origin in the y-direction. There are 40 elements of 5×10^{-5} m height for the fine mesh and 10 elements of 2×10^{-4} m height for the coarse mesh. Symmetry conditions were applied for the 4 boundaries of the computational domain.

2.2 Diatom

The diatom block of the input deck focuses on construction of the bodies of material that make up the problem. Here the initial model is a symmetric 2-D plate impact experiment between 2 copper plates. The plates are infinite in the y-direction and measure 0.005 m in the x-direction. They travel across a gap of 0.0003 m toward each other at 500 m/s each until impact.

2.3 Particles

The continuum solution for this problem is evaluated using the standard CTH code, and it is to be compared with the version of CTH that uses the MPM (CTH with MPM) particle solution. The particles are distributed 3 per cell in the x and y directions and completely represent the copper plates described in the diatom for the particle runs. The particles are capable of

transporting the full state of the material at any specific particle location, but the equation of state (EOS) is evaluated on the background grid. The particles can also analyze multiple material pressures and temperatures with the MMP4 option enabled in this portion of the input deck.

2.4 Equation of State

The EOS used to analyze the problem is the Mie-Gruneisen EOS. The strength of the copper is taken from the Johnson-Cook material parameter database with a Poisson's ratio of 0.3, density of 8950 kg/m^3, and a sound speed of 3560 m/s.

2.5 Tracers

Eight tracers are originally placed along the lower symmetry boundary of the left copper plate in all of the simulations. These tracers point to the locations along the body on which resultant data will be saved, recorded, and later plotted. Recorded variables on the tracers include time, stress, position, pressure, temperature, and density. Each of these values is recorded every 10 ns during the simulation.

In addition to using an appropriate EOS and placing tracers, it was also necessary to compute the analytical equilibrium pressure for this plate impact. This calculation establishes a standard baseline around which computational agreement can be met. This pressure was evaluated using Eq. 2. It multiplies the density, ρ, of the copper plate with the longitudinal wave speed, C_L, and velocity, V, of the plate.[5] An equilibrium pressure of 2.1×10^4 MPa was calculated.

$$P = \rho * C_L * V \; . \tag{2}$$

Not only should the numerically calculated peak pressure value result in an answer on the order of the analytic solution (see Eq. 2), but it should also exhibit a waveform like the one shown in Fig. 1. In Fig. 1 a continuum impact of 2 copper plates has taken place, and the resulting wave has a relatively smooth high-pressure response as it propagates through the plates.

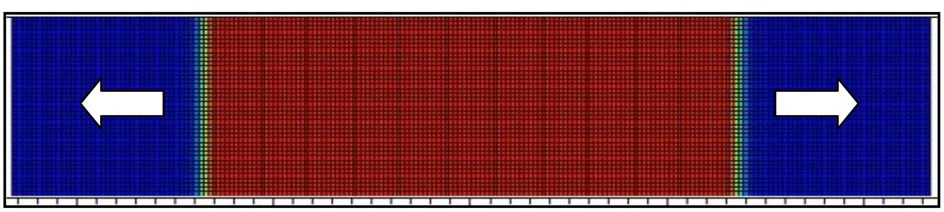

Fig. 1 A continuum pressure contour plot as the impact wave travels after plate impact

3. Results and Discussion

3.1 Plate Contact

It is immediately evident that CTH with MPM is vulnerable to one of the inherent problems with current particle methods: void/particle mixed cell issues. Inspecting the pressure contours from CTH for the initial test shows that the 2 copper plates are not entirely coming into contact (Fig. 2). However, particles away from the impact face experience a pressure increase indicative of impact. The mixed cells at the interface of the 2 plates contain both particles and void space. An investigation into this part of the result will be discussed in more depth for a less complicated problem later in this report.

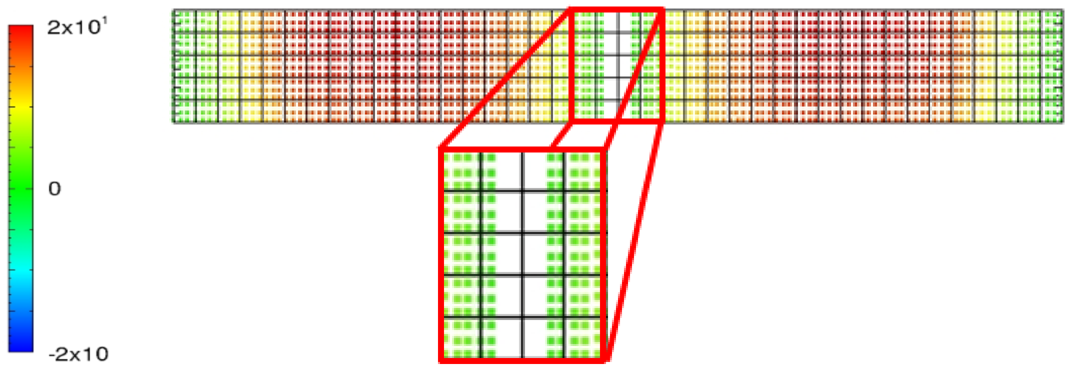

Fig. 2 Pressure impact image from CTH, where the red indicates particle areas of high pressure, and the green indicates areas of zero pressure (scale units in gigapascals)

Upon further investigation, it was also discovered that the particles at the impact face were at zero pressure despite the impact having already taken place, as shown by the green markers in Fig. 2. This particular issue may be linked to the superposition of the particle and background grid pressures discussed previously. Determining why particles are indicating zero pressure at the impact face requires further investigation, but the issue associated with the void gap between the plates is mitigated by physically closing the gap within the problem setup. The plates are placed directly next to one another and move toward each other for impact.

3.2 Lowered Pressure and Mesh Resolution

With the void gap issues having been noted and avoided, it is now possible to continue the original comparison between the particle method of CTH with MPM and continuum CTH. Even though 8 tracers were placed along the left plate within the model, only tracer 4 will be used for data comparison within this report for simplicity. This tracer is located near the middle of the left plate's horizontal width, and it is indicated by the yellow circle within the key of the following figures. The trends discussed for this tracer are assumed to be indicative of the activity at the other tracers.

The left graph in Fig. 3 depicts the pressure impact response at tracer 4 for the coarse mesh compared with the continuum model. For this calculation the response of the particle method is well below that of the continuum solution with an approximate 17% difference in peak pressure value. It is also important to note that the continuum solution's equilibrium pressure value is approximately equal to the analytical solution, previously calculated as 2.08×10^4 MPa. The fine mesh pressure result comparison shown in the right graph of Fig. 3 has better agreement with the continuum solution with only a half percent difference in peak pressure; however, its rise time is much slower, leading to a pressure difference of 15% after the initial rise. Direct comparisons between the 2 mesh resolutions for CTH with MPM are shown in Fig. 4. This result indicates that the solutions from these 2 simulations are not identical. There is approximately a 14% difference in peak pressure values between the 2 resolution models. Additionally, neither of these particle results exhibits the more step-like increase, plateau, and step decrease in pressure obtained using continuum CTH.

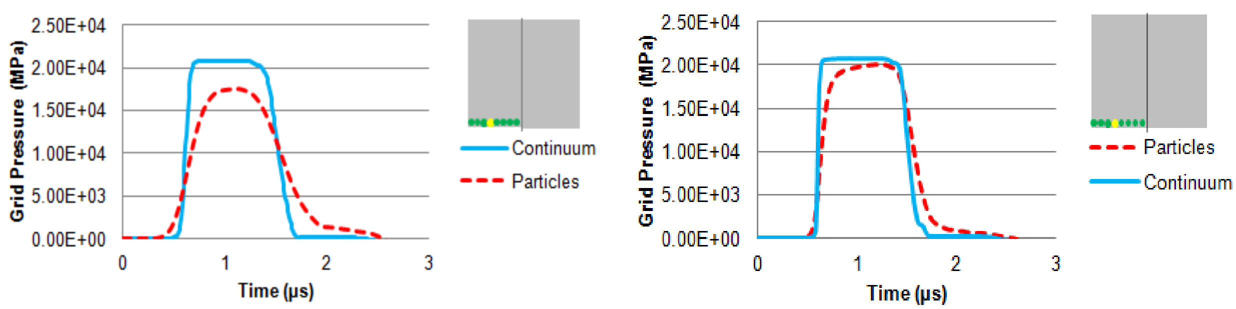

Fig. 3 (Left) Coarse mesh and (right) fine mesh continuum comparisons

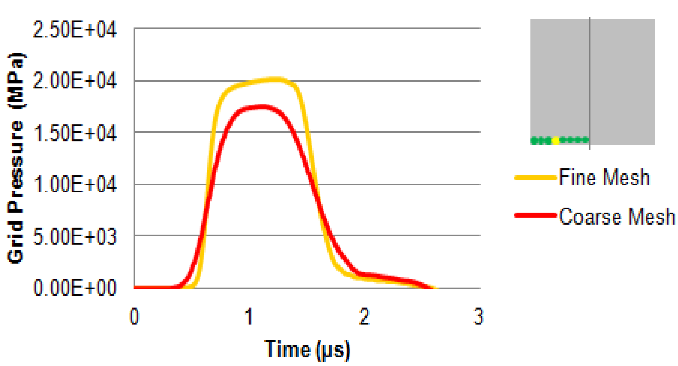

Fig. 4 Mesh resolution comparison shows disagreement

3.3 Tracer Location

The results from tracer 4 at both mesh resolutions are generally below the continuum result. In order to investigate any influence from the boundary conditions, the group of 8 tracers was shifted vertically up. Now instead of taking resultant data from the lower symmetry boundary of the left plate, we gather it from the middle line of the left plate's geometry. This change should

not greatly affect the resultant data from the tracers, but as Fig. 5 shows, the shift causes a noticeable increase in impact pressure by approximately 7%. This indicates that there are boundary condition effects on marker tracers placed on the lower symmetry boundary. This is not observed using continuum CTH.

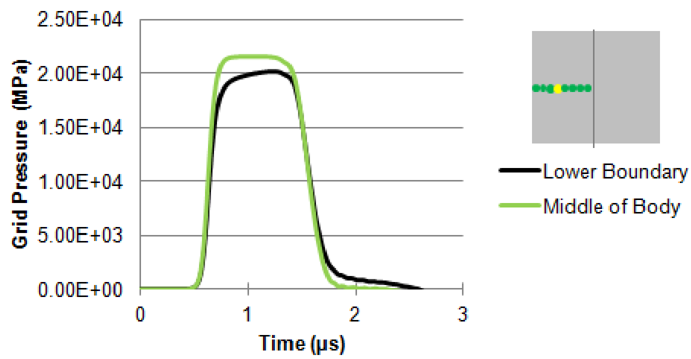

Fig. 5   Tracer 4 pressure comparison based on location

3.4 Raised Pressure

The change in pressure output for tracer 4 as a result of its change in position requires a reevaluation of the original comparison between CTH with MPM and continuum CTH. This time we focus on the results of the fine mesh since it more closely matches the continuum results. Figure 6 shows that the increase in pressure response obtained by tracer relocation has placed the particle method pressure slightly above the continuum result by approximately 4%. This near reversal of the original pressure discrepancy can be qualified further only by investigating the behavior of the particle method specifically, without the coupling to the continuum grid through Eq. 1.

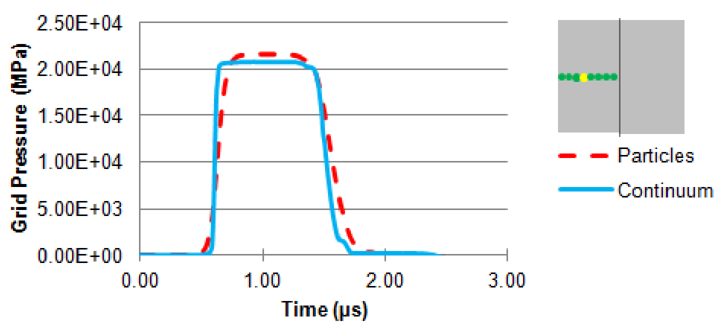

Fig. 6   Fine mesh continuum comparison after the change in tracer location

3.5 Uintah: A Particle Code

To gain additional insight into the performance of the CTH with MPM particle method, a second code is used with the current plate impact problem. Uintah is a pure particle code developed at the University of Utah, and it differs from CTH in that it does not factor in a continuum grid pressure in its momentum equation.[6] The original symmetric impact across a gap problem is built

within Uintah's environment, and the results are analyzed to elucidate what is causing the pressure discrepancy with CTH with MPM.

First, the issue of the mixed cells halting visible plate contact was examined. This behavior can be explained by the method by which particle codes move bodies like the copper plates within the mesh. Uintah allows the plates to initially move toward each other by compressing the void space in between them. This method of resolving the void works well until mixed cells containing both particles and void are encountered just before "physical" impact. Since the particle code applies the same deformation rate onto copper particles and void within any cell, the individual particles within these mixed cells are compressed just like void space. The stress on these particles increases until the average stress on their cells equals the equilibrium pressure signaling to the code that impact has now occurred. Essentially, the code believes that the plates have come in contact even though there is still void space between them.

The gap issue was again sidestepped by setting the 2 plates directly next to each other for the next Uintah simulation. Fig. 7 shows that after the impact of the 2 plates, the resulting waveform is not quite smooth. There is noticeable ringing occurring as the wave propagates through the plates. A more in-depth investigation into this code's particle behavior is necessary.

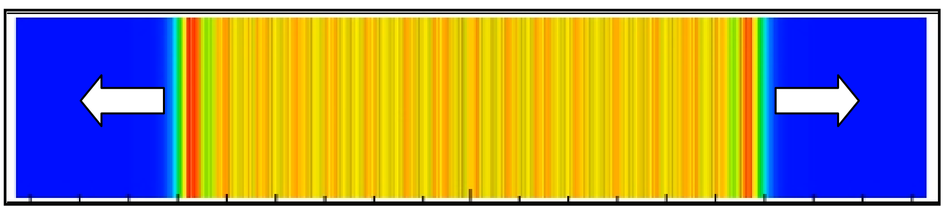

Fig. 7 Pressure contour from Uintah shows ringing as the impact wave travels outward

To begin, 27 tracers are placed at consecutive particle locations in the wake of the impact wave at 0.3 µs after impact. The pressure response of these tracers shows that after the shock passes, 2 particles in a given cell achieve a similar stress level while the final particle falls well above or below in stress. It seems as though the large shock caused by the plate impact raises the stress so quickly with respect to the mesh size that some particles comprising the plate bodies within a cell are not able to reach the final equilibrium pressure state before being pushed into an adjoining cell. However, in this new cell the existing 2 particles have already achieved their final state either at a much higher or lower pressure. The result is a set of high and low pressures that combines to create the correct average pressure. As this effect propagates outward from the impact face, it results in the ringing seen in the pressure plot from Uintah in Fig. 7.

Placing tracers in the same locations for the same time step in CTH with MPM's input deck yielded similar pressure ringing results as obtained with Uintah. The 2 sets of data were then plotted for graphical comparison. The scatter plot of Fig. 8 shows that ringing in CTH with MPM is still apparent, but it has been lessened to some degree. The smoothing of the CTH with MPM results may be a result of the superposition of the pressure values taken from the individual

particles and the background grid through Eq. 1. This mixing of particle and continuum pressure is not done in Uintah. Although the comparison of Uintah as a particle method brought about an unexpected result, further inspection of the particle code's output brought more insight into what may be happening within the particle implementation of CTH.

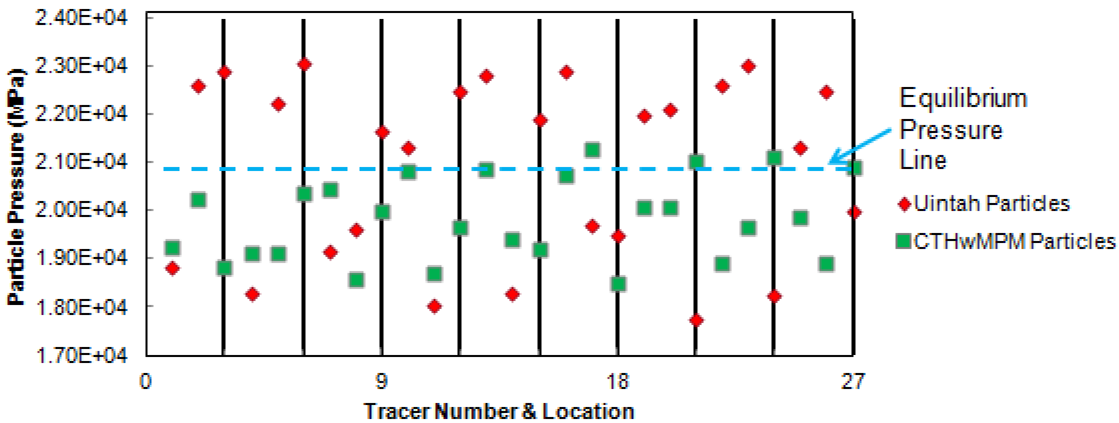

Fig. 8 Individual particle pressure within consecutive cells after plate impact for Uintah and CTH with MPM

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4. Summary and Conclusions

Several issues have been identified within the new implementation of the material point method for the historically continuum-based hydrocode CTH. The current MPM implementation within CTH exhibited the same lack of mixed cell void closure between impacted bodies as Uintah. Boundary condition effects on particle output were discovered upon changing tracer locations within the model. When the resolution of the mesh was changed from coarse to fine, the pressure response from CTH with MPM approached the CTH continuum solution. This mesh sensitivity may indicate that a high level of simulation resolution is necessary with this particle implementation in order to achieve the stress field resolution given by the traditional continuum method. Also, particles appeared to exhibit zero pressure values at the impact face as well as noticeably varied values within a single cell after impact. A number of these concerns revolve around the addition of variables evaluated at the particle and background grid levels within CTH with MPM's solution algorithm. Further research into this implementation will be required to gain a fundamental understanding of how this averaging method couples to particle models. Continued development of CTH with MPM will hopefully solve the problems encountered during the application of this 2-D plate impact problem and eventually much more challenging mechanics scenarios.

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